High Precision Diffractometers for X-ray Advanced Investigations

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Abstract

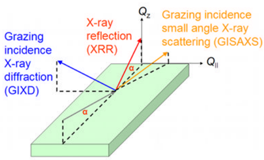
The specific development of a research instrument for X-ray advanced investigations (GISAXS, GIXD, and XRR) working in a synchrotron facility is presented. The innovative product is a versatile *diffractometer* which can be used for *heavy* and *medium* duty tasks enabling to use a large pallet of additional devices for the characterisation of materials in interactions with various controllable environments. In a standard *modular approach*, two multiaxis positioning systems are built on 2+3 circles principle from a combination of several *Positioning modules (Pm)* and *Positioning units (Pu)* - heavy load and high precision Goniometers(G)&Translation tables(T). The total budget of motion errors must be within of small spheres (‘spheres of confusion’).The methodology to obtain and manage them is presented.

Introduction

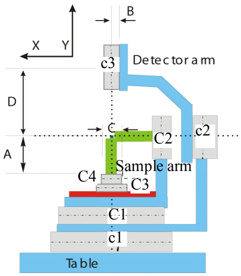
A *synchrotron* [1] is a dedicated facility for the production of X-rays for research and industry. The progresses in micro and nano science are strong related with the actual and further results coming from here. By using *diffraction* [2] technique - a powerful tool to characterise materials, the actual modern work as Grazing Incidence X-ray diffraction (GIXD), Grazing Incidence Small Angle X-ray Scattering (GISAXS) and reflectivity (XRR) aim to provide relation between the microscopic and macroscopic structures at the interfaces - solid/solid, solid/liquid, solid-gas, etc. Among *scientific applications* are thin films, multilayers of metals and semiconductors, soft matter/ polymers, lubrication, tissue engineering or catalysis. The equipments working here [3] e.g. diffractometers are built especially for this purpose. A successfully collaboration work has been recently accomplished ([4], [5]) and consisted in to develop at I07/DLS [6] new beam line two diffractometers - medium (Dm1) and heavy (Dm2) duty tasks, respectively.

1 Working Principle

There are a large number of actual diffractometers' configurations. However, the *basic principle* is almost the same. A *Diffractometer (Dm)* must materialize the motions between the detector (D) and the sample (S) relative to the incoming and refracted/scattering/ reflected X beam. In order to obtain reliable data for the atomic or molecular samples planes, in a fast and reliable mode, the geometry must perform several interconnected motions, as precise as possible.In a *2+3 circle* machine [7], the basic motions consist in: a) *sample motion which is* providing the desired 3D orientation for the sample relative to the incoming beam(C1, C2 circles) and b) *detector motion* positioning the detector head relative to the incoming & diffracted/ scattered X-ray beam taking in to account the sample center(c1,c2,c3 circles). For horizontal scattering (HSc) two more motions (circles C3&C4) are added (Fig.1b).



a)



b)

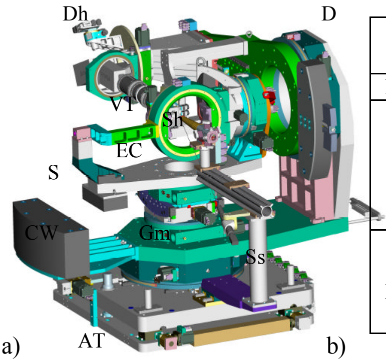
Motion	Type (circle)	Travel [°]	Res. [m°]	Run-out [μm]	Speed [°/s]	Seetling [s]	Acc. [m°]
S	C1	α : 180	0.1	10	5	0.5	1
	C2	ω : 360		5	8	0.1	
	C3(HSc)	χ :+/-20	0.2	10	5	0.5	
	C4(HSc)	θ : 360	0.1	5	8	0.1	
D	c1	γ : -20/+190	0.2	10	5	0.5	
	c2	δ :-20/+190					
	c3	υ: 360				0.1	

Fig. 1 Difractometers working principle: a) fundamentals and b) kinematics

Other *auxiliary motions* are: a) fine sample manipulation (3-6 dof) and b) detectors head adjustment (Tr. and Rot-c4). The investigations are done in two Experimental Hutches (EH). In EH1, the Dm1 is using *medium* load environmental instruments (e.g. baby chamber, etc) in both horizontal /50kg & vertical positions/30kg. In EH2 the Dm2 manipulates *large&heavy* in-situ (e.g.UHV) horizontally/500kg instruments. The detectors weight is max. 50 kg.

2 Design Concept

Both equipments must perform the same basic motions (detector & sample), but with different sample/environments (loads) and circumstance (horizontal/vertical). An innovative design solution has been adopted at a resonable costs. In a standard modular approach, the *Fine alignment* module (Euler Cradle, or Hexapods [8]) will be attached to the basic common *Positioning modules* (Pm)–detector (D) and sample (S) depending of the task (vertical/horizontal scattering). Each Pm is built on a serial combination of standard or special *Positioning Units* (Pu) using heavy load and high precision rotation - Goniometers(G) and/or Translational tables(T), Fig./Tab.2.The Euler Cradle (EC) sub-module consists in two Pu–circles C5(Chi) and C6(Phi).



a) b)

Pm		M	Pu	Stiff [µrad/Nm]	Acc. [“][µm]
B	AT	Rx,Y	6200s	0.05	8/10
S	Arm	C1,2	G430	0.07	10
	HSc	C3	S5202	0.05	8
		C4	G440	0.07	10
	EC	C5,6	EC512	0.1	30
	Head	XYZ	5102/4	0.01	5
D	Arm	c1,c2	G480	0.02	10
	Head	c3	G420	0.2	12
		c4	G409	6	15
		c5,c6	EC511	0.1	30

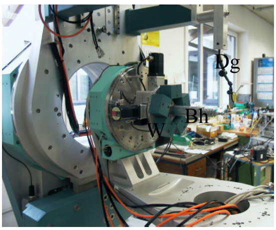
Fig. 2 Full equiped Diffractometer (Dm1): a) Pro-E overview and b) main components

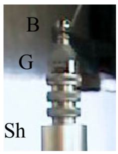
In order to align the Dm relative to the incoming beam, an *alignment base* (AB) has been conceived on Parallel Kinematics Mechanisms (PKM) principle. It consists from a stiff base and a 2dof high precision movable platform(Y,Rx) actuated by four powerful actuators each of two coupled. Basic and specific static and dynamic calculations have been performed regarding the stiffness for both, the basic components (Pu) and sub-assemblies (Pm) in order to assure the necessary stability of motions. When necessary, the counterweights (CW) have been added.

3. Accuracy

The *errors* from the misalignment of the detector and sample displacements have been identified as most important leading to significant errors in computation of final microscopic geometries. A *systematic approach* has been applied in order to manage them inside of an acceptable *Sphere of Confusion* (SOC). Mainly, it started with: 1.

design phase - a) by choosing Pu with adequate accuracy e.g. G/X3 and b) by including the possibility to adjust it (e.g.supports, plates, screws, etc); then, 2. in the manufacturing-a) machining and b) assembly phases, the individual(Pu), or (sub)modules (Pm)) have been carefully checked against the design parameters. Calibration was also necessary for some sensors(e.g. tape). Through the specific positioning-standard or special techniques the geometrical (e.g. straightness, parallelism, etc) and motion (e.g. repeatability, backlash, wobble, etc) type errors have been identified, registered and corrected (if, possible). In this purpose, standard (dial gages, etc) and dedicated instruments (e.g. interferometers, testing stand, etc) were extensively used. The final *motions accuracy* (SoC) have been determined separately and for full travel and load for the main Pm (detector & sample) by using a calibrated*Ballhead*(Bh)-Shaft(Sh)/12mmBall(B)-Sphericity0.1µm(G5/KGM)+ Gonio (G) and *dial gage* (Dg), Fig/Tab.3.

a) 

b) 

3σ values

c)

Pm	C	SoC* [µm]
S	C1&C2	30
D	c1&c2	50
*EC	C5&C6	20

Fig.3 Measurements Tests: a) Set up b) Ball head and c) Values

Conclusion

A multipurpose multiaxis positioning system has been designed as a tool for fast and reliable X-ray advanced investigations. It was conceived on the accumulated experience and the actual developments in precision positioning technology inside of the *design for precision* concept featuring the flexible manipulation of heavy loads with high precision during complex motions.

References

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